About the Training Course:

The training course for the workshop has been designed to provide the theoretical background as well as a hands-on approach to Molecular Docking and Virtual screening. The workshop will also cover the use of different softwares and will focus on Chem-informatics based methods for lead identification and optimization.

Workshop Topics include:

- Basic principles of Homology Modeling
- Methods and Advances in computer aided drug design
- Approaches in Target selection and refinement for docking studies
- Identidication and evaluation of Binding Pocket / Active site
- Docking approches in virtual screening and Lead idenitfication
- Modeling the unknown proteins for docking studies
- Pharmacophore modeling and virtual screening of novel compounds
- Refinement of novel leads using ADME prediction
- Similiraty and disslimiaraity based methods in lead identification
- 3D-QSAR Modeling and Lead optimization
- Biologics Design and Protein engineering

Level of Participants:

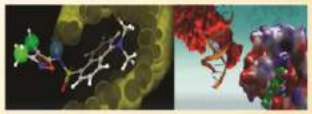
Eligibility qualification of participants:

Participants shall have at least Master's degree in any discipline of Biological Sciences and have a working knowledge of computer applications.

Academicians/Scientists/Research Scholars can participate.

Registration Fee: Rs. 1000/-

Number of Participants: 25



How to apply:*

Application (form can be downloaded using http://ucb.uk.gov.in/wp-content/uploads/2015/07/Short-term-Training-Proforma.pdf) for participation along with biodata duly forwarded by the competent authority of the institute/university where the candidate is presently working may be sent to the Course Coordinator before 31st December, 2016 at the following email addresses (anujbioinfo91@gmail.com, vinod@schrodinger.com) (application via E-mail will be preferred).

The Collaborating Institutes

The above programme is being organized by Dolphin (PG) Istitute of Biomedical and Natural Sciences, Dehra Dun in collaboration with some of the premier, Nationally and Internationally renowned Schrodinger INC and Uttarakhand Council for Biotechnology, Dehradun, Uttarakhand.

Schrodinger INC

Schrödinger INC is the scientific leader in developing state-of-the-art chemical simulation software for use in biotechnology, pharmaceutical and materials science research. Schrodinger is a world class molecular modelling, drug design, and materials science software multinational company. This is working in the area to improve human health and quality of life through development, distribution, and application of advanced computational methods that transform the way scientists design therapeutics and materials. This is pushing the boundaries of drug discoveries with unyielding commitment to continually improve the underlying science and to find new and innovative ways to deploy new technologies for maximal effects. (www.schrodinger.com)

Uttarakhand Council for Biotechnology (UCB)

Uttarakhand Council for Biotechnology is formed to deploy, use, utilise and leverage biotechnology as an effective tool for catalysing accelerated economic growth of Uttarakhand by substantially harnessing and converting its bio-wealth into economic wealth. This council is an autonomous body of Government of Uttarakhand and is working under the guidance of apex body of UCB and functioning as "Nodal Agency" of Department of Biotechnology, Govt. of India, New Delhi for Biotechnology education, research and development in the state of Uttarakhand. (www.ucb.uk.gov.in/)

Dolphin (PG) Institute of Biomedical and Natural Sciences (DIBNS)

DIBNS is committed to academic excellence, healthy standards in co-curricular practices, socially relevant activities, and courses leading to employment and entrepreneurship and continuous progress of the institution. The Institute is affiliated to H.N.B. Garhwal Central University, Srinagar-Garhwal (Uttarakhand) and is also approved and recognized by the State Govt. of Uttarakhand.. The institute is accredited by NAAC and listed u/s 2(f) by UGC. (www.dolphininstitute.in)

3-Day Workshop on

" Workshop Cum Hands-on-Training on Molecular Docking, Virtual Screening & Computational Biology"

10-12 January, 2017

Course Coordinator

Mr. Anuj Kumar
Bioinformatician
Uttarakhand Council for Biotechnology (UCB),
Dehradun-248007

Co-Course Coordinator

Dr. Pritesh Bhat & Mr. Vinod D
Senior Applications Scientist,
Schrödinger INC

Workshop Details

Time	Workshop Topics
Day 1	
1 9.00 to 9.30	Registration
2 9.30 to 11.00	Inaugural
11:00 to 11:30	**Tea Break**
3 11.30 to 12.30	Computational methods and advances in the discovery of small drug designing: Advanced methods to improve virtual screening enrichments. Examples of success stories: Clinical candidates designed using modeling methods. *Presentation*
4 12:30 to 1:15	Selection and refinement ofcrystal structure of target for SBDD; Preparation of ligands for SBDD: Includes selection of PDB structures (target structures) and explanations about the pitfalls in structures and how to refine the structures for SBDD. *Presentation and Hands-on*
01:15 to 2:00	**Lunch Break**

Time	Workshop Topics
5 2.00 to 2.45	Binding site analysis and its importance in Structure based lead identification and optimization: *Presentation and Hands-on*
6 2.45 to 3.45	Recent Developments in Docking Scoring Functions: Docking studies of human P2Y12 receptor inhibitors Structure Based Virtual screening of novel human P2Y12 receptor. *Presentation and Hands-on*
3.45 to 4.00	**Tea Break**
7 4.00 to 5.00	Exercise on modeling the compounds using Docking *Exercise*
Day 2	
8 9:30 to 10.30	Homology modeling of unknown targets: case study with kinase receptor: Homology modeling of MK5 (mitogen-activated protein kinase [MAPK]-activated protein kinase 5): Starting with the selection of sequence, searching the proper homologus template, model building and refinement. Further validation of final model. Advances in Homology Modeling of GPCRs. *Presentation and Hands-on*
10.30 to 11.30	Post Docking analysis: Selection of hits from virtual screening results a) Fingerprint calculations, Data clustering b) Analysis of virtual screening results and selection of hits based clustering, pose filter, SIFT c) MM-GBSA and other accurate method of binding free energy calculations *Hands-on*
11.30 to 11.45	**Tea Break**
9 11.45 to 12.30	Method in achieving the Protein flexibility upon ligand binding (INDUCEDFIT): Case study with MK5 receptor *Presentation and Hands-on*
12:30 to 1:15	**Lunch Break**
10 1:15 to 3.15	Pharmacophore modeling, QSAR and virtual screening of Anti-cancer compounds: Case study with AT1 receptor inhibitors: Identification of common pharmacophore, scoring and validation of pharmacophore, virtual screening of database with diverse compounds. *Presentation and Hands-on*
3.15 to 3.20	**Tea Break**

Time	Workshop Topics
11 3.30 to 4.15	Exercise on homology modeling *Exercise*
Day 3	
12 9.30 to 11.30	Use of Hydration Energetics for Lead Optimization - WaterMap: Extracting thermodynamic information about the solvating water and enumerating the local statistical thermodynamic properties of water solvating the receptor. Case studies on successful designing of selective compounds using WaterMap. *Presentation and Hands-on*
10:30 to 10:45	**Tea Break**
13 11:30 to 12:30	Protein-Protein Docking Protein-protein docking and building complex of Trypsin-trypsin inhibitors Understanding protein-protein interface using Schrodinger PPI tool *Presentation and Hands-on*
12:30 to 1:15	**Lunch Break**
14 1.15 to 2.45	Computational protein engineering for enhancing the binding affinity and properties a) Residue scanning and affinity maturation to identify suitable amino-acids for higher affinity b) Cysteine scanning for increasing the stability of the biologics c) Prediction of the post-translation sites in biologics d) Protein-aggregation predictions *Presentation and Hands-on*
2.45 to 3.15	**Tea Break**
15 3.15 to 05.00	Question & Answers/Revision

PATRONS

Mr. Arvind Gupta
Chairman, DIBNS

Dr. M. K. Nautiyal
Director, UCB

Dr. Raghu Rangaswamy
Schrodinger INC

CONVENORS

Dr. Shailja Pant
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Dr. Arun Kumar
Director, DIBNS

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Deptt. of Biotechnology, DIBNS

Joint Organising Secretary
Mr. Vipul Garg
Deptt. of Biostatistic & Computer, DIBNS

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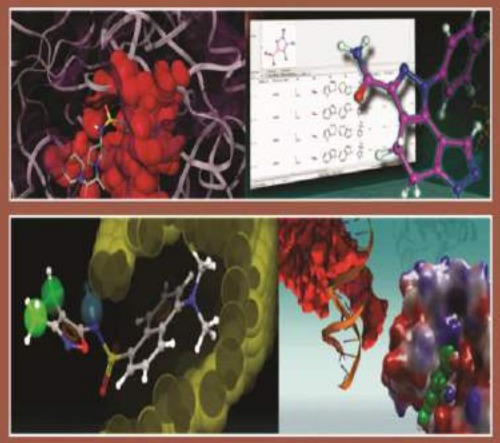
Dr. Upendra Kumar
Er. Rohit Kumar
UCB

Workshop Cum Hands-on-Training on Molecular Docking, Virtual Screening & Computational Biology

10-12 January, 2017



Organized by:

Department of Biotechnology

Dolphin (PG) Institute of Biomedical & Natural Sciences, Dehradun-248007
Accredited by NAAC, listed by UGC u/s. 2(f)

In collaboration with

Uttarakhand Council for Biotechnology
Uttarakhand

Schrodinger INC